Research Toward High Performance Epitaxial and Low-temperature $Cu(In,Ga)Se_2$ Solar Cells

A. Rockett, D.X. Liao, and C.M. Mueller
University of Illinois, Department of Materials Science and Engineering,
1-107 Engineering Sciences Building, MC-233, 1101 W. Springfield Ave., Urbana, IL 61801

ABSTRACT

The CIGS research effort at the University of Illinois represents a three-pronged approach to understanding and solving some of the most critical issues in CIGS device. These three prongs are: (1) development of a basic understanding of the issues limiting performance in CIGS devices, (2) advancing the performance of the devices through single crystal epitaxial layers for integration into high-performance cells, and (3) developing novel growth processes that will allow lower deposition temperatures necessary to multijunction devices. This paper presents an approach for CIGS/GaAs and CIGS/Ge heterojunction solar cells for multijunction high-efficiency devices. In addition, application of ionized physical vapor deposition to low-temperature deposition of CIGS is described. The two projects will be coupled and results from one used to enhance progress in the other as part of the Beyond the Horizon and High Performance PV programs now starting.

1. Introduction

Photovoltaic devices based on $Cu(In,Ga)Se_2$ (CIGS) have the highest performance of any thin film technology. However, the possibilities for even higher performances are significant. Multijunction devices involving CIGS either in conjunction with III-V compound semiconductors (GaAs and related materials) or various Cu chalcopyrite compounds ($CuGaSe_2$, $CuInS_2$, or others) remain to be exploited. The projects described here take two approaches to the study of such devices -- novel processing methods required for multijunction devices, and direct application of the existing methods for deposition to multijunction epitaxial solar cells. These new projects are just beginning at the University of Illinois under the Beyond the Horizon and High Performance Photovoltaics programs funded by the National Renewable Energy Labroatory. The former focuses on developing a novel low-temperature deposition process for production of CIGS. This will be necessary in any application where a CIGS device is to be fabricated on a temperature-sensitive existing junction. The latter involves growth of CIGS epitaxial layers on GaAs and Ge substrates and demonstration of the performance of resulting devices for application with III-V materials. These two projects are briefly summarized below.

2. Ionized Physical Vapor Deposition for CIGS Devices

Under this new program, we will develop a unique next-generation method for low-temperature deposition of CIGS based on the ionized physical vapor deposition (IPVD) method.[1,2] This technique has been shown to dramatically reduce required deposition temperatures in other thin film coatings. It supplies energy to the growing film surface though the working gas rather than by heating the substrate.

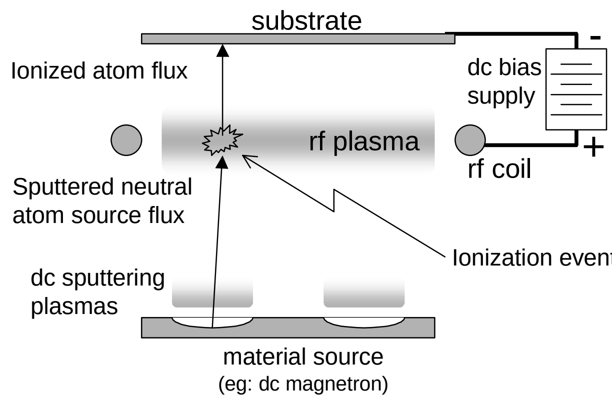

Figure 1: The basic IPVD process.

The basic process is shown schematically in Figure 1. An rf plasma near the substrate ionizes up to 80% of the species in the gas phase.[1] A dc bias voltage (typically 0 to 25 eV) applied between the rf coil and the substrate determines the energy for particles striking the growth surface. The threshold energy for displacement cascades in solids leading to formation of vacancies and interstitials is ~25 eV. Bias below ~50 V keeps the energy transferred to surface atoms below the threshold necessary to damage the film. With 80% of particles striking the growth surface having 10,000 times the thermal energy (i.e. 25 eV), surface atomic mobilities are greatly enhanced and the heat input needed to maintain a given film quality is reduced. Furthermore, the accelerated particles include a number of inert gas species which further contribute to surface adatom motion and film growth. This technique has been used to deposit a variety of films at reduced temperatures. We anticipate a 100-400°C reduction in needed deposition temperature of CIGS epitaxial or polycrystalline layers while retaining device-quality material. We expect to see significantly altered incorporation probabilities for some of the elements in the process, especially an increased Se incorporation rate.

3. CIGS For Multijunction High Performance Devices

As part of the High-performance PV initiative, we are developing CIGS as a narrow-gap component of multijunction solar cells. We currently plan to participate in both the single crystal epitaxial and polycrystalline high performance cell programs. In previous efforts, we have developed a well-characterized and reproducible method for deposition of single-crystal epitaxial layers of $Cu(In,Ga)Se_2$ alloys on GaAs substrates of each of the three major surface orientations, (111), (100), and (110). The technique,[c.f. Refs 3,4] consists of sputtering Cu or Cu-Ga and In targets in Ar gas and simultaneously evaporating molecular Se (and/or S) from an effusion cell or cells.

The present work will begin with a detailed study of the electrical properties of CIGS-GaAs heterojunctions. This is critical to application of CIGS in high efficiency cells for two reasons. First, because the only way to produce a two-contact multijunction solar cell involving CIGS is to use one of the surrounding semiconductors as the heterojunction partner. Therefore, it is necessary to establish the performance of junctions of candidate materials with the CIGS. Second, because the CIGS epitaxial layers are high-quality single crystals, growth of multilayer structures will be possible. Such growth is required in current designs of non-mechanically-stacked high efficiency devices where the 1.0 eV gap device is surrounded both above and below by additional devices. Our preliminary studies will concentrate on demonstration of solar cells based on p-CIS/n^+-GaAs and p-CIS/n-Ge heterojunctions.

Other aspects of the program will include study of methods to control interdiffusion of elements across the heterojunction and low-temperature deposition processes, which will reduce the chance of damage to previously-fabricated III-V heterojunction solar cells. This portion of the program will be closely coupled to the beyond-the-horizon portion of the program, described above.

Finally, we will supply epitaxial layers of CIS on GaAs to NREL for use as substrates for test growth experiments for deposition of III-V semiconductor layers on the CIS films.

These efforts correspond largely to the focus of the single-crystal high-performance program at NREL. We will, however, also be collaborating with the polycrystalline high performance project through supply of materials and growth of device structures. In particular, we will use low-temperature growth to deposit additional junctions on previously grown solar cell layers to test multijunction structures.

4. Thin Film Partnership

While we have, as yet, no indication of funding under the thin film partnership, should this program be funded we will be analyzing solar cell materials gathered from a wide variety of sources by transmission electron microscopy. The objective is to determine the microstructural and microchemical nature of a good CIGS solar cell and how to distinguish it from a poor solar cell. This will assist in optimizing cell performance. This work will be coupled with intensive modeling of device performances, probably based on the AMPS computer code to draw a direct correlation between cell performance and microstructure.

Acknowledgements

The work is being conducted in collaboration with the National Renewable Energy Laboratory and the Institute for Energy Conversion at the University of Delaware, whose help we greatly appreciate.

REFERENCES

[1] C.A. Nichols, S.M. Rossnagel, S. Hamaguchi *J. Vac Sci Techn* B 14(5), 3270 (1996).

[2] S.M. Rossnagel *J. Vac Sci Techn* B 16(6), 3008 (1998), and S.M. Rossnagel *J. Vac Sci Techn* B 16(5), 2585 (1998).

[3] David J. Schroeder, Gene D. Berry, and A. Rockett, *Applied Physics Letters* **69** (26), 1 (1996).

[4] L. Chung Yang, L.J. Chou, A. Agarwal, and A. Rockett, "Single Crystal and Polycrystalline $CuInSe_2$ by the Hybrid Sputtering and Evaporation Method," 22nd IEEE Photovoltaic Specialists Conference, Las Vegas, October 7-11, 1991 (Institute of Electrical and Electronics Engineers, New York, 1991), p 1185.

[5] D. Liao and A. Rockett, *J. Appl. Phys.*, submitted.